FILE 'HOME' ENTERED AT 15:05:23 ON 22 FEB 2007

=>

=> file casreact
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST .

FILE 'CASREACT' ENTERED AT 15:05:38 ON 22 FEB 2007 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE CONTENT:1840 - 18 Feb 2007 VOL 146 ISS 8

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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> Uploading C:\Program Files\Stnexp\Queries\10565829.str

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:06:06 FILE 'CASREACT'

SCREENING COMPLETE -2340 REACTIONS TO VERIFY FROM 229 DOCUMENTS

2340 VERIFIED 100.0% DONE

1 HIT RXNS

1 DOCS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS:

43904 TO

PROJECTED ANSWERS:

1 TO

L2

1 SEA SSS SAM L1 (1 REACTIONS)

=> d

ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN

RX(9) OF 28

REF: Journal of the American Chemical Society, 106(9), 2687-92; 1984

=> s 11 ful

FULL SEARCH INITIATED 15:06:28 FILE 'CASREACT'

SCREENING COMPLETE - 66499 REACTIONS TO VERIFY FROM

4719 DOCUMENTS

100.0% DONE 66499 VERIFIED 69 HIT RXNS

26 DOCS

SEARCH TIME: 00.00.09

26 SEA SSS FUL L1 (69 REACTIONS)

=> d 13 1-26

ANSWER 1 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(2) OF 7

REF: Tetrahedron: Asymmetry, 17(15), 2299-2305; 2006

NOTE: enzymic, stereoselective, >99% ee

CON: 23 hours, 70 deg C, 200 mbar

L3 ANSWER 2 OF 26 CASREACT COPYRIGHT 2007 ACS on STN RX(15) OF 17

Chemistry--A European Journal, 2006, 12(1), 225-232; NOTE: biotransformation, enzymic, stereoselective, yield depends on

catalyst activator

CON: 17 hours, room temperature

ANSWER 3 OF 26 CASREACT COPYRIGHT 2007 ACS on STN L3

-RX(3) OF 9

REF: PCT Int. Appl., 2005095629, 13 Oct 2005
NOTE: biotransformation, enzymic(Novozym 525L used), alternate preparation also described, K2CO3/enzyme batch can be recovered

and reused at least three times, stereoselective

24 hours, 70 deg C CON:

L3 ANSWER 4 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(6) OF 180

Tetrahedron: Asymmetry, 16(15), 2575-2591; 2005

5 minutes, 50 deg C

L3 ANSWER 5 OF 26 CASREACT COPYRIGHT 2007 ACS on STN RX(13) OF 25

Me CH-Me +
$$F_3$$
C-CH₂-O-C-Pr-n $\frac{\text{Subtilisin, Et3N,}}{\text{S:174501-64-5}}$

REF: Green Chemistry, 6(9), 471-474; 2004 NOTE: stereoselective, enantioselective, biotransformation, enzymic,

85% ee

CON: 6 days, room temperature

L3 ANSWER 6 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(5) OF 20

REF: Tetrahedron: Asymmetry, 16(9), 1603-1610; 2005 NOTE: biotransformation, enzymic, stereoselective, alternate preparations also described

CON: 24 hours, 70 deg C, 205 mbar

L3 ANSWER 7 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 19

$$N$$
 CH_2
 OMe
 OMe
 OH
 OH

- 1. CH2Cl2
- 2. Pyridine
- 3. Butanoyl chloride
- 4. Water

RX(3) OF 19

REF: PCT Int. Appl., 2005030763, 07 Apr 2005
NOTE: last stage inverse addn.
CON: STAGE(1) room temperature -> 0 deg C
 STAGE(2) 0 deg C
 STAGE(3) 0 deg C; 0 deg C -> room temperature; 4 hours,

room temperature STAGE(4) 0 deg C

L3 ANSWER 8 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

 PhCH (Me) OH, Ph Acetophenone, o-Xylene i-PrO-C-Pr-n 2. Lipase Pr-n Me (step 1) 4. Al isopropoxide 96%

REF: PCT Int. Appl., 2005014509, 17 Feb 2005

NOTE: biotransformation, enzymic [lipase; Novozym 435 (Candida

antarctica)]; stereoselective; third stage distn. of isopropanol

and butyrate

CON: STAGE(1) room temperature, 1 atm

STAGE(2) room temperature -> 70 deg C, 65 - 70 mbar STAGE(3) 2 hours, 70 deg C, 65 - 70 mbar STAGE(4) 4 hours, 70 deg C

L3 ANSWER 9 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 29

1. C:470688-18-7, t-BuOK, THF, PhMe PhCH (Me) OH, Subtilisin, Na2CO3, Pr-n (step 2) THF 95%

PCT Int. Appl., 2005009935, 03 Feb 2005

NOTE: stereoselective

STAGE(1) room temperature; 1 hour, room temperature STAGE(2) room temperature; 72 hours, room temperature

L3 ANSWER 10 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 13

1. Subtilisin, R:9004-95-9, Pyridine, Water PhCH (Me) OH, C:470688-18-7, Me Pr-n t-BuOK, Na2CO3, 98% THF (step 2)

Journal of the American Chemical Society, 125(38), 11494-11495; REF:

NOTE: optimization study, optimized on solvent, stereoselective,

stereoselectivity increased slightly with other acyl donor (TFEB), biotransformation, enzymic

STAGE(1) 5 minutes, room temperature; 12 hours, 35 deg C STAGE(2) 3 days, 25 deg C CON:

ANSWER 11 OF 26 CASREACT COPYRIGHT 2007 ACS on STN L3

RX(3) OF 21

$$\begin{array}{c|c} O & Ph & O \\ \parallel & PhCH \, (Me) \, OH, \quad Fe2O3, \\ HO-C-CH_2-CH_2-CH_3 & \hline{Amberlyst, \, Carbon} & Me-CH-O-C-Pr-n \\ 95\% \end{array}$$

REF: Journal of Molecular Catalysis A: Chemical, 191(1), 141-147;

2003

NOTE: green chem., activated C contg. amberlyst supported cat.

CON: 1.5 hours, reflux

L3 ANSWER 12 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 30

REF: Archiv der Pharmazie (Weinheim, Germany), 334(10), 318-322; 2001

L3 ANSWER 13 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 8

REF: PCT Int. Appl., 2001090396, 29 Nov 2001 NOTE: stereoselective, enzymic, biotransformation

L3 ANSWER 14 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

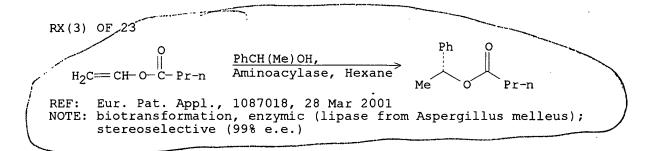
RX(2) OF 2

Ph O | || Me-CH-O-C-Pr-n

REF: Biotechnology and Bioengineering, 74(4), 295-308; 2001 NOTE: biotransformation, enzymic, optimization study

L3 ANSWER 15 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

not goed



L3 ANSWER 16 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

civetic rosolutions
ret DKR.

configet et. RX(2) OF 15 PhCH (Me) OH, Aminoacylase, PhMe

Synlett, (4), 367-370; 1997 NOTE: biotransformation, enzymic, acylase from Aspergillus, stereoselective

L3 ANSWER 17 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

e qta. RX(1) OF 1 PhCH (Me) OH, Subtilisin

Journal of the American Chemical Society, 113(8), 3166-71; 1991 NOTE: Biotransformation: catalyzed by subtilisin

L3 ANSWER 18 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(1) OF 2

$$F_3C-CH_2-O-C-Pr-n$$
 PhCH (Me) OH Me O Pr-n

Acta Chemica Scandinavica, 44(10), 1032-5;

ANSWER 19 OF 26 CASREACT COPYRIGHT 2007 ACS on STN L3

REF: Jpn. Kokai Tokkyo Koho, 01215298, 29 Aug 1989, Heisei
NOTE: Biotransformation: catalyzed by lipase p from pseudomonas sp.; #
Conditions: 1,15 mol educt + trichloro-ethyl butyrate, 100-500 g
cellfree enzyme; in diethyl-ether; 45 h, 25.deg.c

L3 ANSWER 20 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(8) OF 95

448

Journal of Antibiotics, 41(11), 1552-60;

L3 ANSWER 21 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(3) OF 72

Biocatalysis, 2(3), 217-23; 1989 REF:

NOTE: Biotransformation: catalyzed by lipase from candida cylindracea; # Conditions: cellfree enzyme, in org. solvent (cyclohexane),

ANSWER 22 OF 26 CASREACT COPYRIGHT 2007 ACS on STN L3

REF: Journal of Organic Chemistry, 53(23), 5531-4; 1988

L3 ANSWER 23 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

REF: Journal of Organic Chemistry, 53(10), 2374-8; 1988

L3 ANSWER 24 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

REF: Journal of the Chemical Society, Chemical Communications, (2); 114-15; 1987

L3 ANSWER 25 OF 26 CASREACT COPYRIGHT 2007 ACS on STN

RX(4) OF 18

$$Cl_3C-CH_2-O-C-Pr-n$$
PhCH (Me) OH, Et2O
 Me
 O
 $Pr-n$

REF: Journal of the American Chemical Society, 107(24), 7072-6; 1985

RX(9) OF 28

REF: Journal of the American Chemical Society, 106(9), 2687-92; 1984

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE ENTRY

TOTAL SESSION

FULL ESTIMATED COST

2.40

2.61

FILE 'CAPLUS' ENTERED AT 16:59:02 ON 22 FEB 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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=> s 11

L2 2 L1

=> d 12 1-2

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1997:480441 CAPLUS

DN 127:94192

TI Manufacture of optically active $\alpha\text{-alkyl-}2\text{-halobenzyl}$ alcohols and esters by enzymic hydrolysis and their use in manufacture of optically active 3-alkylphthalides

IN Izumi, Taeko

PA Kawaken Fine Chemicals Co., Japan

SO Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PAN.CNT I					
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
			·		
ΡI	JP 09149791	Α	19970610	JP 1995-312372	19951130
PRAI	JP 1995-312372		19951130		
OS	MARPAT 127.94192				

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1996:559620 CAPLUS

DN 125:300725 TI Chemoenzymic synthesis of optically active 3-methyl- and 3-butylphthalides ΑU Izumi, Taeko; Itou, Osamu; Kodera, Keiji CS Dep. of Materials Sci. and Technology, Yamagata Univ., Yonezawa, 992, Japan SO Journal of Chemical Technology & Biotechnology (1996), 67(1), 89-95 CODEN: JCTBED; ISSN: 0268-2575 Wiley PB DT Journal

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

English

LA

SINCE FILE TOTAL ENTRY SESSION 2.83 5.44

FILE 'REGISTRY' ENTERED AT 16:59:31 ON 22 FEB 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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http://www.cas.org/ONLINE/UG/regprops.html

=> s 59517-15-7 L3 0 59517-15-7 => s 59517-15-6 L4 1 59517-15-6 (59517-15-6/RN)

=> d

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 59517-15-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2-hydroxy-1,2-diphenylethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H20 O3

LC STN Files: CA, CAPLUS

FILE 'HOME' ENTERED AT 16:58:30 ON 22 FEB 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:58:39 ON 22 FEB 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3 DICTIONARY FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> s 182742-53-6

L1 1 182742-53-6

(182742-53-6/RN)

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 182742-53-6 REGISTRY

ED Entered STN: 06 Nov 1996

CN Butanoic acid, 1-(2-iodophenyl)ethyl ester, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H15 I O2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (-).

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 7.35 12.79

FULL ESTIMATED COST

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=> s 14

L5 1 L4

=> d

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1976:420732 CAPLUS

DN 85:20732

TI The reaction of diols with aldehydes in the presence of iodine monochloride and t-butanol: a novel diol monoester synthesis

AU Goosen, Andre; McCleland, Cedric W.

CS Org. Res. Lab., Univ. Port Elizabeth, Port Elizabeth, S. Afr.

SO Journal of the South African Chemical Institute (1975), 28(3), 358-64 CODEN: JSACAT; ISSN: 0038-2078

DT Journal

LA English

FILE 'HOME' ENTERED AT 16:50:56 ON 22 FEB 2007

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:51:07 ON 22 FEB 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3 DICTIONARY FILE UPDATES: 22 FEB 2007 HIGHEST RN 922553-43-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\0565829.str

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR

G1 Cy, Hy, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 16:51:26 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 11848 TO ITERATE

16.9% PROCESSED 2000 ITERATIONS

1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 230438 TO PROJECTED ANSWERS: 1 TO

0438 TO 243482 1 TO 264

L2 1 SEA SSS SAM L1

=> d

L2 . ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN

RN 102332-45-6 REGISTRY

ED Entered STN: 26 May 1986

CN Butanoic acid, 1-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)pentyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H21 C12 N3 O2

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s l1 ful

FULL SEARCH INITIATED 16:52:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 237598 TO ITERATE

100.0% PROCESSED 237598 ITERATIONS

272 ANSWERS

SEARCH TIME: 00.00.03

L3 272 SEA SSS FUL L1

=> d 13 1 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260-272

L3 ANSWER 1 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 915297-77-7 REGISTRY

ED Entered STN: 13 Dec 2006

CN Butanoic acid, (1R)-1-[4-(trifluoromethyl)phenyl]ethyl ester (CA INDEX NAME)

FS STEREOSEARCH

MF C13 H15 F3 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 10 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 866365-13-1 REGISTRY

ED Entered STN: 28 Oct 2005

CN Butanoic acid, (1S)-1-(6-methoxy-2-naphthalenyl)ethyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H20 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 20 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 849341-97-5 REGISTRY

ED Entered STN: 27 Apr 2005

CN Butanoic acid, (S)-cyano(6-methoxy-2-naphthalenyl)methyl ester (9CI) (CA

INDEX NAME)

FS STEREOSEARCH

MF C17 H17 N O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 3 REFERENCES IN FILE CA (1907 TO DATE)
- 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 30 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 838841-86-4 REGISTRY

ED Entered STN: 28 Feb 2005

CN Benzenepropanoic acid, 4-methyl- β -(1-oxobutoxy)-, ethyl ester,

 (βS) – (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H22 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 40 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 777005-82-0 REGISTRY

ED Entered STN: 08 Nov 2004

```
CN Butanoic acid, 1-[4-[(1-methylethyl)thio]phenyl]-2-(octylamino)propyl ester, (R*,S*)- (9CI) (CA INDEX NAME)
```

FS STEREOSEARCH

MF C24 H41 N O2 S

CI COM SR CA

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 ANSWER 50 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 682770-98-5 REGISTRY

ED Entered STN: 18 May 2004

CN Benzenepentanoic acid, 2,4-dichloro- β -oxo- δ -(1-oxobutoxy)-, ethyl ester, (δ S)- (9CI) (CA INDEX NAME)

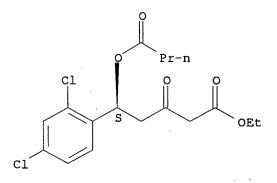
FS STEREOSEARCH

MF C17 H20 C12 O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 60 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 682770-83-8 REGISTRY

ED Entered STN: 18 May 2004

CN Benzenepentanoic acid, β -oxo- δ -(1-oxobutoxy)-, methyl ester, (δS) - (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H20 O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 70 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 682770-71-4 REGISTRY

ED Entered STN: 18 May 2004

CN Benzenepentanoic acid, 4-methoxy- β -oxo- δ -(1-oxobutoxy)-, methyl ester, (δ R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H22 O6

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 80 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 667915-63-1 REGISTRY

ED Entered STN: 26 Mar 2004

CN Butanoic acid, (1R)-1-(4-bromophenyl)-2-(diethoxyphosphinyl)ethyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H24 Br O5 P

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1907.TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 90 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 617713-64-1 REGISTRY

ED Entered STN: 17 Nov 2003

CN Butanoic acid, (1S)-1-(3-hydroxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H16 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 100 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 410093-04-8 REGISTRY

ED Entered STN: 02 May 2002

CN Butanoic acid, (1S)-3-chloro-1-phenylpropyl ester (9CI) (CA' INDEX NAME)

FS STEREOSEARCH

MF C13 H17 C1 O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 110 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 256498-56-3 REGISTRY

ED Entered STN: 23 Feb 2000

CN Benzeneacetic acid, 4-methoxy- α -(1-oxobutoxy)-, methyl ester, (α R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C14 H18 O5

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 120 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 211229-77-5 REGISTRY

ED Entered STN: 15 Sep 1998

CN Butanoic acid, (R)-cyano(pentafluorophenyl)methyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H8 F5 N O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 130 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 182742-53-6 REGISTRY
- ED Entered STN: 06 Nov 1996
- CN Butanoic acid, 1-(2-iodophenyl)ethyl ester, (S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C12 H15 I O2
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (-):

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 140 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 168465-75-6 REGISTRY
- ED Entered STN: 06 Oct 1995
- CN Butanoic acid, 2-azido-1-phenylpropyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C13 H17 N3 O2
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

$$\begin{array}{c|c}
 & N3 \\
 & R & S & O & Pr-n \\
 & Ph & O & O
\end{array}$$

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 150 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 146037-52-7 REGISTRY
- ED Entered STN: 19 Feb 1993
- CN Butanoic acid, 2-azido-1,2-diphenylethyl ester, (R*,R*)- (9CI) (CA INDEX

NAME)

OTHER CA INDEX NAMES:

CN Butanoic acid, 2-azido-1,2-diphenylethyl ester, $(R^*,R^*)-(\pm)$ -

FS STEREOSEARCH

MF C18 H19 N3 O2

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 160 OF 272. REGISTRY COPYRIGHT 2007 ACS on STN

RN 141927-94-8 REGISTRY

ED Entered STN: 19 Jun 1992

CN Benzenepropanoic acid, α -methoxy- β -(1-oxobutoxy)-, methyl ester, (R*,R*)-(-)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H20 O5

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Rotation (-). Absolute stereochemistry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 170 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 134696-85-8 REGISTRY

ED Entered STN: 05 Jul 1991

CN Benzoic acid, 4-(5-heptyl-1,3-dioxan-2-yl)-, 4-[1-(1-oxobutoxy)ethyl]phenyl ester, [2(S)-trans]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H40 O6

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 180 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 134604-21-0 REGISTRY
- ED Entered STN: 28 Jun 1991
- CN Benzoic acid, 4-(octyloxy)-, 4-[1-(1-oxobutoxy)ethyl]phenyl ester, (R)-(9CI) (CA INDEX NAME)
- FS · STEREOSEARCH
- MF C27 H36 O5
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 190 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 130517-86-1 REGISTRY

ED Entered STN: 16 Nov 1990

CN Benzenepropanoic acid, α -azido- β -(1-oxobutoxy)-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Benzenepropanoic acid, α -azido- β -(1-oxobutoxy)-, ethyl ester, (R^*, S^*) -(\pm)-

FS STEREOSEARCH

MF C15 H19 N3 O4

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 200 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 127626-09-9 REGISTRY

ED Entered STN: 15 Jun 1990

CN Butanoic acid, 1-(4'-hydroxy[1,1'-biphenyl]-4-yl)ethyl ester, (+)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H20 O3

SR CA

LC STN Files: CA, CAPLUS

Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 210 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 119838-96-9 REGISTRY

ED Entered STN: 31 Mar 1989

CN Benzoic acid, 4-[1-(1-oxobutoxy)ethyl]-, (+)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN (+)-4-(1-Butyryloxyethyl)benzoic acid

FS STEREOSEARCH

MF C13 H16 O4

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 220 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 118253-91-1 REGISTRY

ED Entered STN: 30 Dec 1988

CN Benzoic acid, 4-[1-(1-oxobutoxy)ethyl]-, 4'-(octyloxy)[1,1'-biphenyl]-4-yl

ester, (+)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C33 H40 O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 230 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 115482-86-5 REGISTRY

ED Entered STN: 30 Jul 1988

CN Butanoic acid, 2-hydroxy-1-phenylethyl ester, (S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H16 O3

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT (*File contains numerically searchable property data)

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 240 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 89378-61-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, (1R)-1-phenylethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Butanoic acid, 1-phenylethyl ester, (R)-

OTHER NAMES:

CN (R)-1-Phenethyl butanoate

CN (R)-1-Phenylethyl butyrate

FS STEREOSEARCH

MF C12 H16 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

25 REFERENCES IN FILE CA (1907 TO DATE)

25 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 250 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 74059-60-2 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzeneethanaminium, N,N,N, α -tetramethyl- β -(1-oxobutoxy)-, iodide, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H26 N O2 . I STN Files: CA, CAPLUS LC(82763 - 01 - 7)CRN

Absolute stereochemistry.

• I-

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 260 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN66681-75-2 REGISTRY

ED Entered STN: 16 Nov 1984

Butanoic acid, 2,2,2-tribromo-1-(4-methylphenyl)ethyl ester, (-)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C13 H15 Br3 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 261 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN . L3

RN66681-71-8 REGISTRY

ED Entered STN: 16 Nov 1984

يؤال الانهوا أزاد وأوارف الدائد الأخطاطية القياس أعبا محلكتك Butanoic acid, 2,2,2-trichloro-1-(4-methylphenyl)ethyl ester, (-)- (9CI) CN (CA INDEX NAME)

FS STEREOSEARCH

MF C13 H15 C13 O2

STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 262 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 66681-67-2 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2,2,2-tribromo-1-(3-chlorophenyl)ethyl ester, (-)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H12 Br3 Cl O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 263 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 66681-63-8 REGISTRY

CN Butanoic acid, 2,2,2-trichloro-1-(3-chlorophenyl)ethyl ester, (-)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H12 C14 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Rotation (-).

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 264 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 66681-53-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2,2,2-trichloro-1-(3,4-dichlorophenyl)ethyl ester, (-)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C12 H11 C15 O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

- L3 ANSWER 265 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN .
- RN 66574-79-6 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN Butanoic acid, 2-[methyl[1-methyl-2-(1-oxobutoxy)-2 phenylethyl]amino]ethyl ester, hydrochloride, [R-(R*,S*)]- (9CI) (CA
 INDEX NAME)
- FS STEREOSEARCH
- MF C20 H31 N O4 . Cl H
- LC STN Files: CA, CAPLUS

CRN (66574-69-4)

Absolute stereochemistry.

● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 266 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 66574-69-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2-[methyl[1-methyl-2-(1-oxobutoxy)-2-phenylethyl]amino]ethyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H31 N O4

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 267 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 66274-02-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzeneethanaminium, N,N, α -trimethyl- β -(1-oxobutoxy)-N-[2-(1-oxobutoxy)ethyl]-, iodide, (R*,R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H34 N O4 . I

LC STN Files: CA, CAPLUS

CRN (792134-37-3)

• I-

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 268 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 66273-97-0 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2-[methyl[1-methyl-2-(1-oxobutoxy)-2-

phenylethyl]amino]ethyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H31 N O4

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.

$$\begin{array}{c|c} n\text{-Pr} & O & Me \\ \hline O & Me & S & O & Pr-n \\ \hline \\ Ph & O & \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 269 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 59517-15-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 2-hydroxy-1,2-diphenylethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H20 O3

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 270 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 55574-22-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 1-(1,3-benzodioxol-5-yl)-2-[4-(2,4-dimethylphenyl)-1-piperazinyl]propyl ester, hydrochloride, (R*,S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H34 N2 O4 . x Cl H

CRN (740745-67-9)

Relative stereochemistry.

●x HCl

L3 ANSWER 271 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN

RN 55545-90-9 REGISTRY

ED Entered STN: 16 Nov 1984

CN Butanoic acid, 1-(1,3-benzodioxol-5-yl)-2-[4-(2,4-dimethylphenyl)-1-piperazinyl]propyl ester, monohydrochloride, (R*,S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H34 N2 O4 . Cl H

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CRN (740745-67-9)

HCl

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- L3 ANSWER 272 OF 272 REGISTRY COPYRIGHT 2007 ACS on STN
- RN 36922-22-2 REGISTRY
- ED Entered STN: 16 Nov 1984
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]methyl]-8-oxo-7-[[(1-oxobutoxy)phenylacetyl]amino]-, monosodium salt, [6R-[6 α ,7 β (R*)]]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C23 H24 N4 O6 S3 . Na
- LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, TOXCENTER
- CRN (782388-23-2)

Absolute stereochemistry.

Na

- 4 REFERENCES IN FILE CA (1907 TO DATE)
- 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)